

Physics of interface: Barrier with correlations and disorder sandwiched between two metallic planes

Sanjay Gupta*

S. N. Bose National Centre for Basic Sciences, Kolkata, India

Tribikram Gupta†

Theoretical Physics Division, Indian association for the Cultivation of Sciences, Kolkata, India

(Dated: March 22, 2011)

A Metal-Disordered Mott insulator-Metal heterostructure is studied at half-filling using unrestricted Hartree Fock method. The corresponding clean system has been shown to be an insulator for any finite on site correlation. Interestingly we find that introduction of explicit disorder induces a metal-insulator transition at a critical value of disorder. The critical value corresponds to the point at which disorder nullifies the effect of onsite correlation. The wavefunctions are found to delocalize by increasing disorder, rendering the system metallic.

PACS numbers: 73.20.-r, 71.27.+a, 71.30.+h, 71.10.Fd, 73.21.b, 73.40.c

INTRODUCTION

The field of heterostructures, has seen tremendous interest in recent times both experimentally[1–3] and theoretically[4–8]. Heterostructures fabricated out of strongly correlated systems, in particular have shown very novel properties. These emergent properties are sometimes very different from the properties of the individual constituent materials. For example the heterostructure of a Mott insulator and a band insulator has been shown to have metallic behaviour[1]. This is due to aggregation of delocalized electrons at the interface of such a heterostructure. On lowering the temperature, the system can even become superconducting[2].

In this paper, we investigate a metal-disordered Mott insulator heterostructure. The corresponding clean case system has recently received lot of theoretical attention and has been variously claimed to be a fragile Fermi liquid[7] which shows metallic character at any finite correlation strength, and a "de facto impenetrable Mott insulator" [6], with highly decaying spectral weight at the Fermi energy. In a recent work we[8] have shown that the clean system is insulating for all finite values of correlation that we could work with. The system was also found to have multiple gaps in the energy spectrum, as a result of charge reconstruction on varying correlations.

An interesting relevant question in this context is the role of disorder on the whole phenomenon. Experimentally heterostructures are fabricated with a certain degree of disorder present in them. The disorder can arise due to non trivial local atomic and electronic structure due to the presence of dangling bonds and incomplete atomic coordination. With these fundamental issues in mind, we have investigated a heterostructure comprising of a metal-disordered Mott insulator-metal sandwich. Very interestingly, we find that the introduction of disorder can generate a metal insulator transition in the region where the corresponding clean system was gapped. This

is because disorder is able to nullify the effect of correlation in a certain range of values and also delocalize the wave functions. The route to metallicity has very close connection to the metallic phase that is stabilised by increasing disorder from a clean Mott insulator, due to the closing of the Mott gap as shown by Aguiar et. al [9], using generalized DMFT methods.

In the system we study here, there is charge reconstruction between the planes and consequent inhomogeneity in the underlying charge landscape. This inhomogeneity was found to be sufficient to render the system insulating even in the gapless state of the clean system. Here we show that disorder is able to negate the effect of correlation over a small range of values and generates a metallic phase.

We work with correlated disorder of the Thue-Morse and Fibonacci type. Correlated disorder has been studied extensively before[10–13]. Theoretical studies of the quasi-periodic systems have shown that in the non-interacting limit the wave function shows a power law localization both in one[14] and two[15] dimensions. A very recent experiment in a 1D quasi-periodic optical lattice[13], where the system was described by an Aubry-Andre Hamiltonian, has shown exponentially localized states(Anderson localization) in the large disorder limit. A theoretical explanation of the above result has been attempted using Fibonacci sequence in 1D [16]

Correlated disorder introduces a certain type of disorder which does not depend on the realisation, but still breaks translational symmetry. Its relevance in capturing the effect of interplay between correlation and disorder has been shown recently by us[17]. The two chosen sequences have been wrapped over the quasi 2D system in the Mott layers.

We use unrestricted Hartree Fock to study the problem as it is able to capture the role of disorder exactly and the effect of spatial variation in the order parameters both in plane and perpendicular to them. The effect of

correlation is captured in a fully self consistent manner. It works very well in higher dimensions at half filling and even in 2D [18] and 1D [19] gives results comparable to QMC and real space renormalization calculations. It cannot however capture the effect of large effective mass renormalization and the evolution of the sharp metallic peak in the spectral function at the Fermi energy.

Model and Method

We now present and discuss our work. We take the barrier of our metal-barrier-metal sandwich to be described by the single-orbital disordered Hubbard model, and the metallic planes by the tight-binding model. The Hamiltonian for the system is

$$\mathcal{H} = \sum_{i\sigma} (\epsilon_i - \mu) n_{i\sigma} - \sum_{ij\alpha\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{i\alpha} U_\alpha (n_{i\alpha\uparrow} - \frac{1}{2})(n_{i\alpha\downarrow} - \frac{1}{2}). \quad (1)$$

Here i, j is the site index. The operator $c_{i\alpha\sigma}^\dagger$ ($c_{i\sigma}$) creates (destroys) an electron of spin σ at site i . We set both the in-plane and the inter plane hopping to be nearest neighbor only, and equal to t . The lattice structure is that of a simple cubic lattice. ϵ_i denotes the site potential at the i th site which follows either a Thue-Morse or a Fibonacci sequence in the barrier planes and are zero in the metallic planes.

A Thue-Morse sequence is generated by following the rule: $A \rightarrow AB$ and $B \rightarrow BA$, where A and B are the two different sites. In our case site B has a higher site potential than site A ($\epsilon_B > \epsilon_A$, $W = \epsilon_B - \epsilon_A$, being the disorder strength). Thue-Morse chain in a particular generation looks like: $ABBABAABBAABABBA...$. The A and B sites are found in equal numbers in any Thue Morse sequence of even entries. The generating scheme of Fibonacci sequence is $A \rightarrow AB$ and $B \rightarrow A$. A typical Fibonacci chain in a particular generation looks like: $ABAABABAABAABABAABABA.....$. Here sites A and B follows a golden mean ratio. These two sequences correspond to two different impurity site concentration in the system. In Thue Morse 50% of the barrier sites are B type, while in Fibonacci the corresponding number is 38%. It is therefore expected that the effect of disorder would be more strong for the Thue Morse disorder compared to the Fibonacci disorder. These sequences have been wrapped over the quasi 2D lattice in the barrier planes. The interaction term is written in a particle-hole symmetric fashion. The chemical potential μ is calculated by demanding that there be exactly N electrons in the problem and is calculated by taking the average of the $N/2$ th and the $(N/2 + 1)$ th energy level. We label the planes by α with $\alpha = m$ or $\alpha = 1$ corresponding to

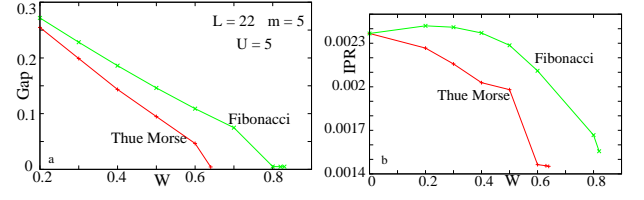


FIG. 1: a. Variation of gap for $U = 5$ with increasing disorder for Thue Morse and Fibonacci sequences. b. IPR with increasing disorder for $U = 5$ for Fibonacci and Thue Morse sequences

the metallic layers. All the other α values in between correspond to the barrier planes. Thus $U_1 = U_m = 0$, while for all other α , $U_\alpha = U$.

In a recent work [8] we had studied the interface of a quasi 2D barrier with onsite correlations sandwiched between two metallic planes and shown that even a very small correlation strength renders the system insulating. The system for very low U behaves like a gapless insulator, while for larger U , the system opens a gap at half filling and then behaves like a gapped insulator. For even higher U , the system shows the presence of multiple gaps. In this work we will fix U to be in the region where the system has opened a single gap. We then turn on the disorder strength from zero and study the evolution of this system.

We use unrestricted Hartree Fock method to address the problem as we do not want to restrict or bias the solutions in any particular manner. The price we pay in the process is the time taken to attain self consistency in the solutions, upto the high precision that we seek. This precision value is 10^{-7} in the square of the density of both up and down electron density. We need to perform about 100 iterations away from the transition point to reach self consistency, while close to the metal-insulator transition point we need to perform more than 1000 iterations to reach the same consistency. For disorder strength even higher than the transition value, it is very difficult to reach self consistency as the numerical solution vacillates between several close lying minima solutions. Hence we avoid this region of parameters in this work. The initial seed that we provide to the system becomes increasingly important as the system approaches the metal insulator transition point. Deep in the Mott insulator regime we find that though the system is not highly sensitive to the initial seed in determining the outcome of the final ground state, a mixed antiferromagnetic seed gives the lowest energy for both Fibonacci and Thue Morse type of disorder. Close to the transition point we find the initial seed that gives the lowest energy is different for the two types of disorder. This is because close to the transition point the effective single particle potential landscape that emerges due to competition between correlation and disorder becomes highly sensitive to the

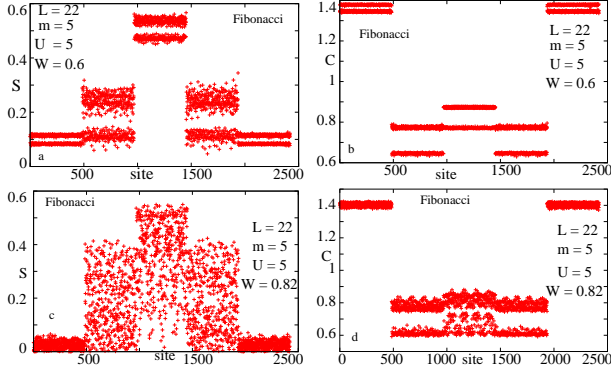


FIG. 2: Spin and charge profiles for Fibonacci type of disorder. a. Spin at each site for $U = 5$ and $W = 0.6$. b. Charge at each site for $U = 5$ and $W = 0.6$. c. Spin at each site for $U = 5$ and $W = 0.82$. d. Charge at each site for $U = 5$ and $W = 0.82$.

concentration and distribution of the impurity sites.

Calculated quantities

We study the effect of increasing W on the gap at half filling, the spin and charge profile and the Kubo conductivity at zero temperature. The charge at a particular site is simply calculated as $C = n_{i,\uparrow} + n_{i,\downarrow}$. The spin at a particular site is given by $S = |(n_{i,\uparrow} - n_{i,\downarrow})|$. The optical conductivity is calculated using the Kubo formula, which at any temperature is given by:

$$\sigma(\omega) = \frac{A}{N} \sum_{\alpha, \beta} (n_{\alpha} - n_{\beta}) \frac{|f_{\alpha\beta}|^2}{\epsilon_{\beta} - \epsilon_{\alpha}} \delta(\omega - (\epsilon_{\beta} - \epsilon_{\alpha})) \quad (2)$$

with $A = \pi e^2 / \hbar a_0$, a_0 being the lattice spacing, and $n_{\alpha} = \text{Fermi function with energy } \epsilon_{\alpha} - \mu$. The $f_{\alpha\beta}$ are matrix elements of the current operator $j_x = it \sum_{i, \sigma} (c_{i+x a_0, \sigma}^{\dagger} c_{i, \sigma} - h.c.)$, between exact single particle eigenstates $|\psi_{\alpha}\rangle$, $|\psi_{\beta}\rangle$, etc, and ϵ_{α} , ϵ_{β} are the corresponding eigenvalues. In this paper, conductivity/conductance is expressed in units of $A = \pi e^2 / \hbar a_0$.

We calculate the ‘average’ conductivity over 3-4 small frequency intervals $\Delta\omega (\Delta\omega = n\omega_r, n = 1, 2, 3, 4)$, and then differentiate the integrated conductivity to get $\sigma(\omega)$ at $\omega = n\omega_r, n = 1, 2, 3, 4$ [17, 20]. The ω_r is taken to be twice the lowest frequency that can be accessed of a finite size lattice ($\omega_r = 2 * D/N$), where D is the bandwidth and N is the total number of sites in the system.

For the quasi 2D geometry taken by us $N = m \times L^2$, where m is the total number of layers (metal + insulator) and L is the total number of sites along both x and y direction, in the numerical work.

Results and Analysis

Our results in this paper corresponds to $U = 5$ in presence of disorder. We have chosen this value as representative of the region where the clean system is a Mott insulator. As we increase the disorder strength, the gap at half filling closes and the system becomes metallic. There is also a gradual delocalization of the wavefunction as the disorder strength is increased. The spin order parameter becomes highly dispersed in each of the planes as the metallic phase is approached. The peak conductivity values are roughly the same for both types of correlated disorder considered in this work.

Fig 1a shows the phenomenon of the gap at half filling, due to correlation, closing due to the presence of disorder. Disorder introduces states at half filling. The concentration of B sites is more for the Thue Morse sequence compared to the Fibonacci sequence. Hence the Thue Morse sequence is able to kill the gap more quickly than the Fibonacci sequence. Thus we see that while the Thue Morse sequence kills the gap to a value less than the finite size spacing at roughly $W = 0.6$, the Fibonacci sequence is able to achieve the same reduction in gap at around $W = 0.82$.

Fig 1b looks at the change in the extent of localization of the wavefunction as we increase the disorder through the Inverse Participation Ratio (IPR). High IPR values indicate higher localization while low IPR values indicate delocalized wavefunctions. The IPR decreases monotonically with increasing disorder, thus indicating that the wave functions become more delocalized. The calculation has been done for both Thue Morse and Fibonacci sequence of disorder. The delocalization process is more rapid for the Thue Morse type and is more gradual for the Fibonacci sequence. We have not been able to go beyond the transition point due to the onset of a glassy phase which makes it very difficult to calculate the correct configuration accurately.

From our previous studies [8] we know that for $m = 5$ which means 3 intervening Mott layers, there is a gap at half filling for $U = 5$ accompanied by the induction of anti ferromagnetic ordering. The Mott layers induces an anti ferromagnetic ordering even in the metal planes. The ordering is non uniform as one moves along the z-axis with the maximum value at the central plane.

Fig 2 and Fig 3 shows the spin and total charge at each site for Fibonacci and Thue Morse type of disorder respectively, for $L = 22$, $m = 5$, $U = 5$. Thus in the figures, the first L^2 sites correspond to the lowest metallic plane, the next L^2 sites correspond to the adjacent Mott plane, the next L^2 to the central layer Mott plane and so on. There is obvious symmetry about the central plane in the spin and charge order parameters.

Fig 2a and 2c show the spin profile for the insulating ($W = 0.6$) and metallic ($W = 0.82$) regime re-

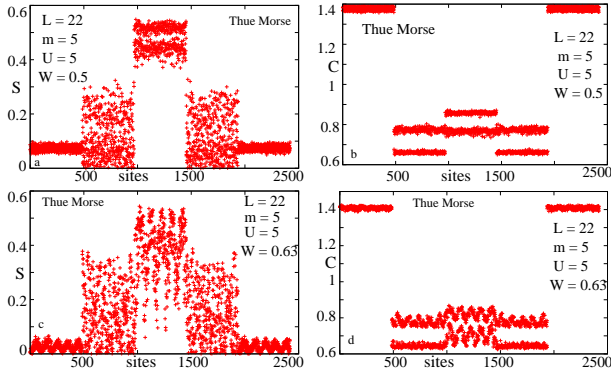


FIG. 3: Spin and charge profiles for Thue Morse disorder. a. Spin at each site for $U = 5$ and $W = 0.5$. b. Charge at each site for $U = 5$ and $W = 0.5$ c. Spin at each site for $U = 5$ and $W = 0.63$. d. Charge at each site for $U = 5$ and $W = 0.63$

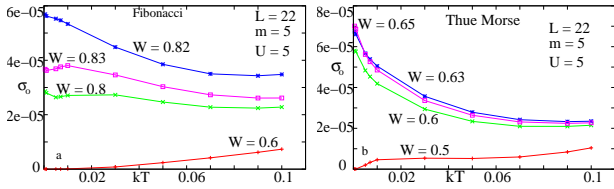


FIG. 4: a. Insulator-Metal-Insulator transition observed with increasing disorder strength of the correlated Fibonacci type.

spectively, while Figs 2b and 2d show the charge profile for the same values of W . Figs 3a and 3c shows the corresponding spin profile for the insulating ($W = 0.5$) and metallic ($W = 0.63$) regime respectively, for the Thue Morse sequence, while Figs 3b and 3d show the charge profile for the same values of W .

We find disorder increases the total charge buildup in the metallic layers. The charge depletion from the Mott layers just adjacent to the metallic planes and the charge accumulation in the metallic planes increases with increasing W . The spin profile becomes totally dispersed for the metallic phase in contrast to a less dispersed profile in the insulating phase.

From the Kubo conductivity plots shown in Figs 4a and 4b we find that as we increase disorder for fixed $U = 5$, the system shows a metal insulator transition (MIT). The conductivity value changes non monotonically with increasing disorder in the metallic phase.

CONCLUSION

A metal-disordered Mott insulator-metal interface heterostructure is studied. A disorder induced metal insulator transition is observed, over a small range of disorder values, in the range where the clean system is gapped.

Sanjay Gupta would like to thank the DST for providing the grant under the project "Electronic states and transport in mesoscopic/nanoscale systems".

* sanjay1@bose.res.in

† trbkrm01@yahoo.co.in

- [1] A. Ohtomo et al., *Nature (London)*, **419**, 378 (2002), *Nature (London)*, **427**, 423 (2004).
- [2] S. Thiel, G. Hammerl, A. Schmehl, C. W. Schneider, and J. Mannhart, *Science*, **313**, 1942 (2006).
- [3] Kenji Yonemitsu, Nobuya Maeshima and Tatsuo Hasegawa, *Phys. Rev. B*, **76**, 235118, (2007)
- [4] W. C. Lee and A. H. MacDonald, *Phys. Rev. B*, **74**, 075106 (2006).
- [5] S. Okamoto and A. J. Millis, *Nature (London)*, **428**, 630 (2004); *Phys. Rev. B*, **70**, 241104(R) (2004); *Phys. Rev. B*, **72**, 235108 (2005).
- [6] R. W. Helmes, T. A. Costi, and A. Rosch, *Phys. Rev. Lett.* **101**, 066802 (2008).
- [7] H. Zenia, J. K. Freericks, H. R. Krishnamurthy, Th. Pruschke, *Phys. Rev. Lett.*, **103**, 116402, (2009).
- [8] Sanjay Gupta, Tribikram Gupta *arXiv 1003.4642* (2004); *Phys. Rev. B*, **70**, 241104(R) (2004); *Phys. Rev. B*, **72**, 235108 (2005).
- [9] Aguiar M. C. O. et. al., *Phys. Rev. Lett.* **102**, 156402 (2009)
- [10] Merlin R. et. al., *Phys. Rev. Lett.*, **55**, (1985) 1768.
- [11] Delahaye J. et. al., *Phys. Rev. B*, **67** (2003) 214201.
- [12] Sanjay Gupta et. al., *Physica B*, **355** (2005) 299; De Brito P. E. et. al. *Phys. Rev. B*, **73** (2006) 014301; Mauriz P. W. et. al., *Phys. Rev. B*, **63** (2001) 184203; Vasconcelos M. S. et. al., *Phys. Rev. B*, **59** (1999) 11128.
- [13] Roati G. et. al., *Nature*, **453** (2008) 895.
- [14] Kohomoto Mahito et. al., *Phys. Rev. B*, **34** (1986) 563;
- [15] Sutherland B., *Phys. Rev. B*, **34** (1986) 3904, *Phys. Rev. B*, **39** (1989) 5834.
- [16] Modugno M., *New J. Phys.*, **11** (2009) 033023.
- [17] Tribikram Gupta and Sanjay Gupta, *Euro Physics Letters* **88**, 17006 (2009).
- [18] Lin H. Q. and Hirsch J. E., *Phys. Rev. B* **35**, 3359 (1987)
- [19] Sanjay Gupta et. al. *Phys. Rev. B* **63**, 125113 (2001)
- [20] Sanjeev Kumar and Pinaki Majumdar, *Europhys. Lett* **65**, 75 (2004)